annotated version

Machine Learning Course - CS-433

Expectation-Maximization Algorithm

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Martin Jaggi
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credits to Mohammad Emtiyaz Khan & Rüdiger Urbanke

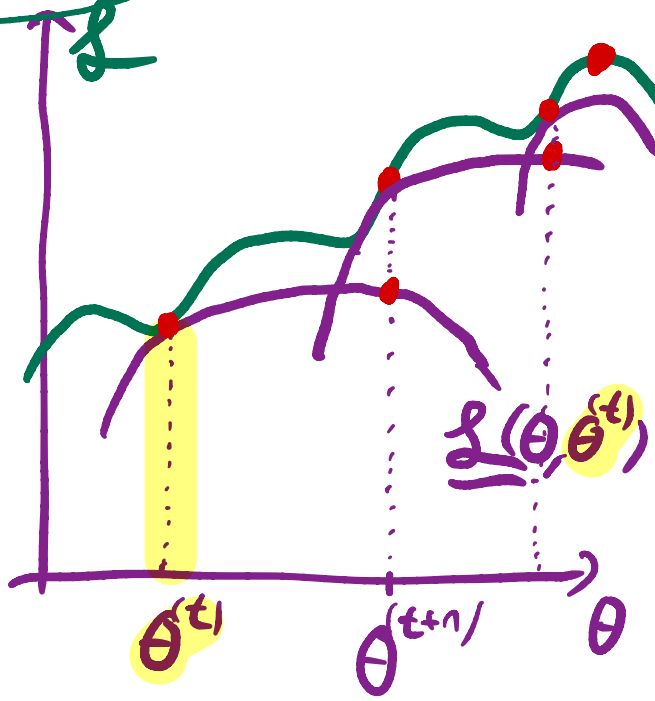
EPFL

Motivation

Computing maximum likelihood for Gaussian mixture model is difficult due to the log outside the sum.

$$\max_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) := \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Expectation-Maximization (EM) algorithm provides an elegant and general method to optimize such optimization problems. It uses an iterative two-step procedure where individual steps usually involve problems that are easy to optimize.



EM algorithm: Summary

Start with $\boldsymbol{\theta}^{(1)}$ and iterate:

1. Expectation step: Compute a lower bound to the cost such that it is tight at the previous $\boldsymbol{\theta}^{(t)}$:

$$\mathcal{L}(\boldsymbol{\theta}) \geq \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) \text{ and } \mathcal{L}(\boldsymbol{\theta}^{(t)}) = \underline{\mathcal{L}}(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t)}).$$

2. Maximization step: Update $\boldsymbol{\theta}$:

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}).$$

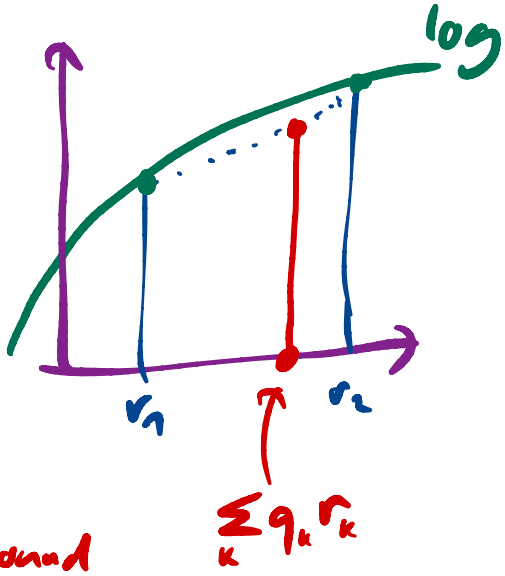
⇔ convexity of -log

Concavity of log

Given non-negative weights q s.t. $\sum_k q_k = 1$, the following holds for any $r_k > 0$:

⇔ Jensen's inequality

$$\log\left(\sum_{k=1}^{K} q_k r_k\right) \geq \sum_{k=1}^{K} q_k \log r_k$$



The expectation step

lower bound

① $\mathcal{L}_n$

$$\log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \geq \sum_{k=1}^{K} q_{kn} \log \frac{\pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{q_{kn}}$$

r_k

$\mathcal{L}_n(\theta, \theta^{(t)})$

② with equality when,

$$q_{kn} = \frac{\pi_k^{(t)} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{k=1}^{K} \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}$$

This is not a coincidence.

$\mathcal{L}_n(\theta^{(t)}, \theta^{(t)}) \doteq \mathcal{L}_n(\theta^{(t)})$

$= \sum_k q_{kn}^{(t)} \log(\dots r_k \dots)$

$= \sum_{k=1}^{K} \frac{\pi_k^{(t)} \mathcal{N}(x|\mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_{k'} \pi_{k'} \mathcal{N}(x|\dots)} \log \frac{\pi_k \mathcal{N}(x|\mu_k, \Sigma_k)}{\pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \sum_{k'} \pi_{k'} \mathcal{N}(x|\mu, \Sigma)}$

$= \log \sum_{k'} \pi_{k'} \mathcal{N}(x|\mu, \Sigma) \cdot 1$

$= \mathcal{L}_n(\theta^{(t)})$

The maximization step

Maximize the lower bound w.r.t. $\boldsymbol{\theta}$.

$$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \sum_{k=1}^{K} q_{kn}^{(t)} \left[\log \pi_k + \log \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]$$

Differentiating w.r.t. $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k^{-1}$, we can get the updates for $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$.

$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$$

$$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} (\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})^\top}{\sum_n q_{kn}^{(t)}}$$

For π_k, we use the fact that they sum to 1. Therefore, we add a Lagrangian term, differentiate w.r.t. π_k and set to 0, to get the following update:

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_{n=1}^{N} q_{kn}^{(t)}$$

+ k-means as a special case

Summary of EM for GMM

Initialize $\boldsymbol{\mu}^{(1)}, \boldsymbol{\Sigma}^{(1)}, \boldsymbol{\pi}^{(1)}$ and iterate between the E and M step, until $\mathcal{L}(\boldsymbol{\theta})$ stabilizes.

1. E-step: Compute assignments $q_{kn}^{(t)}$:

$$q_{kn}^{(t)} := \frac{\pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{k=1}^{K} \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}$$

$\propto c \cdot \exp(-\|x_n - \mu_k\|^2 / \sigma^2)$ ...

$\sigma \to 0$ → $\begin{cases} 1 & k \text{ closest to } x_n \\ 0 & \text{otherwise} \end{cases}$

2. Compute the marginal likelihood (cost). = k-means assignment = z_{kn}

$$\mathcal{L}(\boldsymbol{\theta}^{(t)}) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k^{(t)} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})$$

3. M-step: Update $\boldsymbol{\mu}_k^{(t+1)}, \boldsymbol{\Sigma}_k^{(t+1)}, \pi_k^{(t+1)}$.

$q_{kn} = z_{kn}$

$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$$

= k-means update

$$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} (\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})^\top}{\sum_n q_{kn}^{(t)}}$$

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_n q_{kn}^{(t)}$$

← # points assigned to cluster

k-means and spherical

If we let the covariance be diagonal i.e. $\boldsymbol{\Sigma}_k := \sigma^2 \mathbf{I}$, then EM algorithm is same as K-means as $\sigma^2 \to 0$.

σ: width of cluster

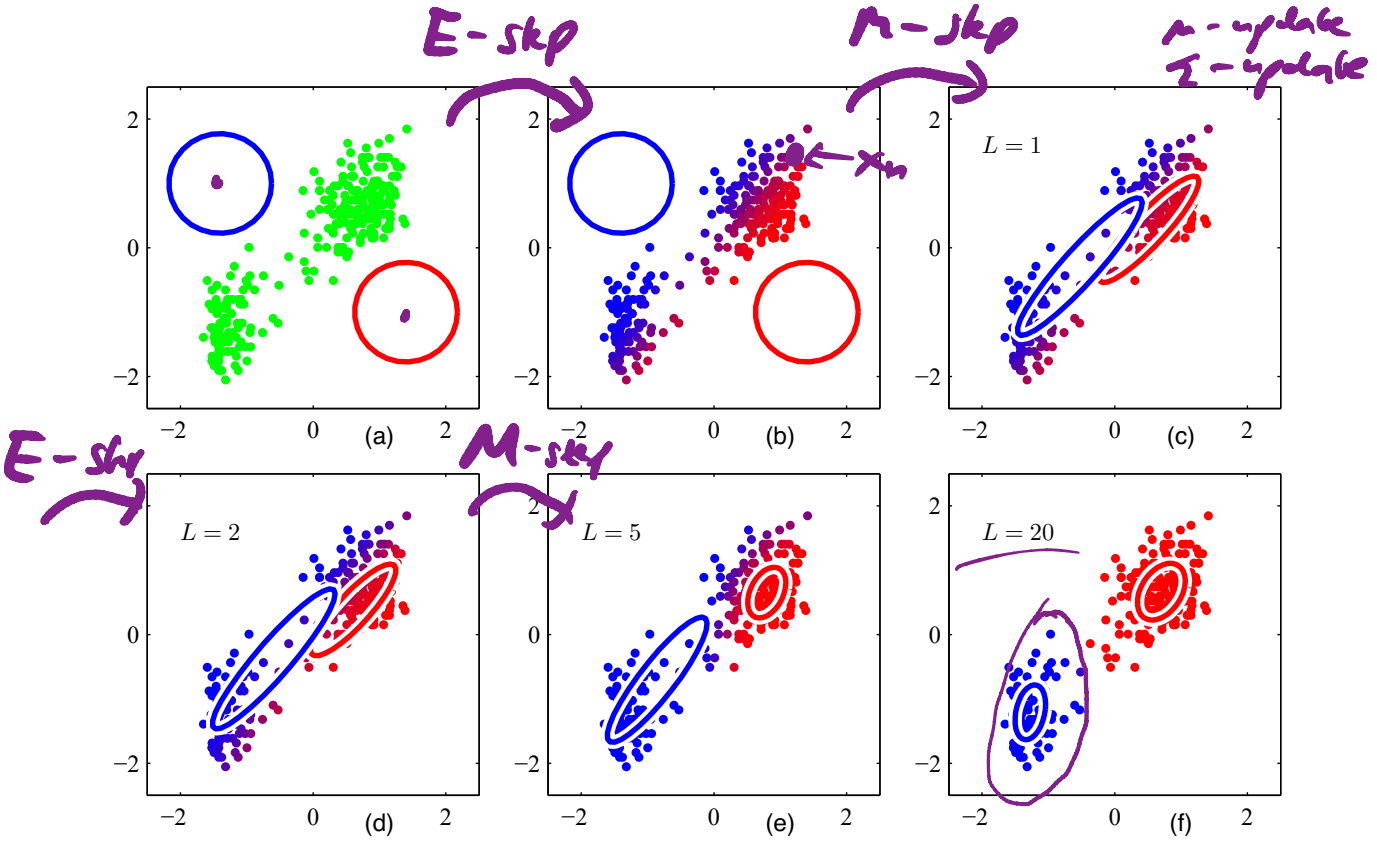


Figure 1: EM algorithm for GMM

Posterior distribution

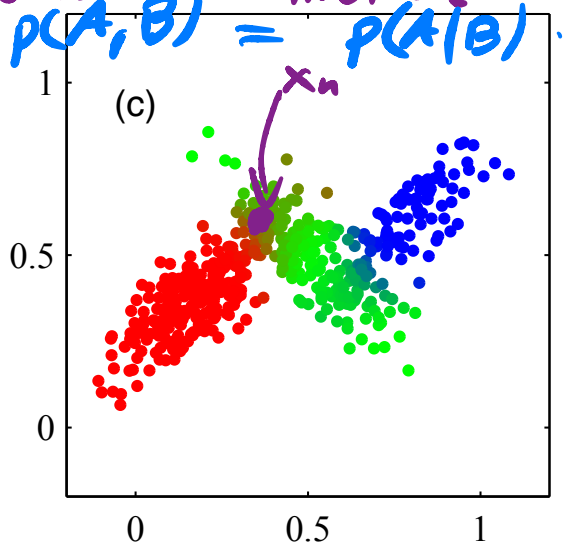
We now show that $q_{kn}^{(t)}$ is the posterior distribution of the latent variable, i.e. $q_{kn}^{(t)} = p(z_n = k \mid \mathbf{x}_n, \boldsymbol{\theta}^{(t)})$

$$p(\mathbf{x}_n, z_n|\boldsymbol{\theta}) = p(\mathbf{x}_n|z_n, \boldsymbol{\theta})p(z_n|\boldsymbol{\theta}) = p(z_n|\mathbf{x}_n, \boldsymbol{\theta})p(\mathbf{x}_n|\boldsymbol{\theta})$$

likelihood · prior = posterior · marginal

joint $p(A,B) = p(A|B) \cdot p(B) = p(B|A) \cdot p(A)$ — Bayes Rule

$$p(z_n = k|x_n, \theta) = \frac{\text{prior} \cdot \text{likelihood}}{\text{marginal lik.}} = \frac{\pi_k \cdot \mathcal{N}(x|\mu_k, \Sigma_k)}{\sum_{k=1}^{K} p(z_n = k|\theta)\, p(x_n|z_n = k, \theta)} = \frac{\pi_k \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_k \pi_k \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k)} = \gamma_{kn}$$



EM in general

Given a general joint distribution $p(\mathbf{x}_n, z_n|\boldsymbol{\theta})$, the marginal likelihood can be lower bounded similarly:

The EM algorithm can be compactly written as follows:

$$\boldsymbol{\theta}^{(t+1)} := \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{p(z_n|\mathbf{x}_n,\boldsymbol{\theta}^{(t)})}\left[\log p(\mathbf{x}_n, z_n|\boldsymbol{\theta})\right]$$

Another interpretation is that part of the data is missing, i.e. $(\mathbf{x}_n, z_n)$ is the "complete" data and z_n is missing. The EM algorithm averages over the "unobserved" part of the data.